

NAME

GLStrGen.pl - Generate structures for Glycerolipids (GL)

SYNOPSIS

GLStrGen.pl GLAbbrev|GLAbbrevFileName ...

GLStrGen.pl [-h, --help] [-o, --overwrite] [-r, --root rootname] [-w, --workingdir dirname] <arguments>...

DESCRIPTION

Generate Glycerolipids (GL) structures using compound abbreviations specified on a command line or in a CSV/TSV Text file. All the command line arguments represent either compound abbreviations or file name containing abbreviations. Use *-m*, *--mode* option to control the type of command line arguments.

A SD file, containing structures for all GL abbreviations along with ontological information, is generated as an output.

SUPPORTED ABBREVIATIONS

Current support for GL structure generation include these main classes and sub classes:

o Monoradylglycerols

- . Monoacylglycerols
- . Monoalkylglycerols
- . Mono-(1Z-alkenyl)-glycerol

o Diradylglycerols

- . Diacylglycerols
- . Alkyl, acylglycerols
- . Dialkylglycerols
- . 1Z-alkenyl, acylglycerols

o Triradylglycerols

- . Triacylglycerols
- . Alkyl, diacylglycerols
- . Dialkyl, monoacylglycerols
- . 1Z-alkenyl, diacylglycerols

OPTIONS

-h, --help

Print this help message

-m, --mode *Abbrev|AbbrevFileName*

Controls interpretation of command line arguments. Two different methods are provided: specify compound abbreviations or a file name containing compound abbreviations. Possible values: *Abbrev* or *AbbrevFileName*. Default: *Abbrev*

In *AbbrevFileName* mode, a single line in CSV/TSV files can contain multiple compound abbreviations. The file extension determines delimiter used to process data lines: comma for CSV and tab for TSV. For files with TXT extension, only one compound abbreviation per line is allowed.

Wild card character, *, is also supported in compound abbreviations.

Examples:

```
Specific structures: MG(16:0/0:0/0:0) DG(18:1(11E)/16:0/0:0)
                    TG(16:0/16:0/18:1(9Z))
Specific structures: MG(0-16:0/0:0/0:0) DG(0-16:1(1Z)/16:0/0:0)
                    TG(0-20:0/16:0/18:1(9Z))
Specific possibilities: DG(18:*/16:0/0:0) DG(18:1(*)/16:0/0:0)
                      DG(*:*(9Z)/16:0/0:0)
                      DG(*:*(9Z)/*:*(11E)/0:0)
All TG possibilities: *(*:*/*:*/*:*) or *(*/*/*)
All MG, DG and TG possibilities: "MG(*:*/0:0/0:0)" "DG(*:*/*:*/0:0)"
                                "DG(*:*/0:0/*:*)" "TG(*:*/*:*/*:*)"
```

Along with wild card character, +/- can also be used for chain lengths to indicate even and odd lengths at sn1/sn2/sn3 positions; additionally > and < qualifiers are also allowed to specify length requirements. Examples:

```
Odd and even number chains at sn1 and sn2: TG(*+:/*-:*/*:*)
Odd and even number chains at sn1 and sn2 with length longer than
10 and 20: TG(*+>10:*/*->20:*/*:*)
```

Default sn2 stereochemistry is R. However, abbreviation format also supports these additional stereochemistry specifications for sn2 position: S; U - unknown; rac - racemic mixture. Examples:

```
MG(16:0/0:0/0:0)[rac] - racemic mixture
DG(18:1(11E)/16:0/0:0)[S] - sn2 stereochemistry is S instead of
default R
TG(16:0/16:0/18:1(9Z))[U] - sn2 stereochemistry is unknown
```

To generate all isomers for specific chains in DG and TG, use of iso designation is also supported. Stereochemistry specification support is not available with isomeric structure generation.

Examples:

```
DG(18:1(11E)/16:0/0:0)[iso2] - Two isomeric structures
TG(16:0/16:0/18:1(9Z))[iso3] - Three isomeric structures
TG(16:0/18:0/18:1(9Z))[iso6] - Six isomeric structures
```

Additionally, all isomeric structures can also be generated by explicit specification of chains at different positions:

```
DG(18:1(11E)/16:0/0:0) DG(16:0/18:1(11E)/0:0)
TG(16:0/16:0/18:1(9Z)) TG(16:0/18:1(9Z)/16:0)
TG(18:1(9Z)/16:0/16:0/)
```

Wild card chain abbreviations are supported with sn2 stereochemistry but not with isomer abbreviation.

-o, --overwrite

Overwrite existing files

-r, --root *rootname*

New file name is generated using the root: <Root>.sdf. Default for new file names: GLAbbrev.sdf, <AbbrevFileName>.sdf, or <FirstAbbrevFileName>1To<Count>.sdf.

-w, --workingdir *dirname*

Location of working directory. Default: current directory

EXAMPLES

On some systems, command line scripts may need to be invoked using *perl -s GLStrGen.pl*; however, all the examples assume direct invocation of command line script works.

To generate a GLStructures.sdf file containing a structure specified by a command line GL abbreviation, type:

```
% GLStrGen.pl -r GLStructures -o "MG(16:0/0:0/0:0)"
```

To generate a GLStructures.sdf file containing structures specified by a command line GL abbreviations, type:

```
% GLStrGen.pl -r GLStructures -o "MG(16:0/0:0/0:0)"
"DG(18:1(11E)/16:0/0:0)" "TG(16:0/16:0/18:1(9Z))"
```

To generate a GLStructures.sdf file containing structures specified by a command line GL abbreviations with specific stereochemistry, type:

```
% GLStrGen.pl -r GLStructures -o "MG(16:0/0:0/0:0)[rac]"
"DG(18:1(11E)/16:0/0:0)[S]" "TG(16:0/16:0/18:1(9Z))[U]"
```

To generate a GLStructures.sdf file containing all isomeric structures specified by a command line GL abbreviations, type:

```
% GLStrGen.pl -r GLStructures -o "DG(18:1(11E)/16:0/0:0)[iso2]"
"TG(16:0/16:0/18:1(9Z))[iso3]" "TG(16:0/16:0/18:1(9Z))[iso6]"
```

To enumerate all possible GL structures and generate a GLStructures.sdf file, type:

```
% GLStrGen.pl -r GLStructures -o "**(/**/*)"
```

or

```
% GLStrGen.pl -r GLStructures -o "**(*:*/*:*/*:*)"
```

or

```
% GLStrGen.pl -r GLStructures -o "**(*:*(*)/*:*(*)/*:*(*))"
```

To enumerate all possible Monoradylglycerols structures and generate a MonoGLStructures.sdf file, type:

```
% GLStrGen.pl -r MonoGLStructures -o "MG(*/*:0/0:0)"
```

To enumerate all possible Diradylglycerols structures and generate a DiGLStructures.sdf file, type:

```
% GLStrGen.pl -r DiGLStructures -o "DG(*/*/*:0)"
```

To enumerate all possible Monoradylglycerols structures with one double bond on acyl chain and generate a GLStructures.sdf file, type:

```
% GLStrGen.pl -r MonoGLStructures -o "MG(*:1/0:0/0:0)"
```

To enumerate all possible Monoradylglycerols structures with even chain lengths and generate a

GLStructures.sdf file, type:

```
% GLStrGen.pl -r MonoGLStructures -o "MG(*+:/0:0/0:0)"
```

To enumerate all possible Diradylglycerols structures with odd chains longer than 10 at sn1 and even chains longer than 18 at sn2, and generate a DiGLStructures.sdf file, type:

```
% GLStrGen.pl -r DiGLStructures -o "DG(*->10:*/*+>18:*/0:0)"
```

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SEE ALSO

GPStrGen.pl

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